

Quantum dot ground state energies and spin polarizations: soft versus hard chaos

Denis Ullmo,^{1,2} Tatsuro Nagano,³ and Steven Tomsovic³

¹*Laboratoire de Physique Théorique et Modèles Statistiques (LPTMS), 91405 Orsay Cedex, France*

²*Department of Physics, Duke University, Durham, North Carolina 27708-0305, USA*

³*Department of Physics, Washington State University, Pullman, WA 99164-2814, USA*

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We consider how the nature of the dynamics affects ground state properties of ballistic quantum dots. We find that “mesoscopic Stoner fluctuations”, that arise from the residual screened Coulomb interaction, are very sensitive to the degree of chaos. It leads to ground state energies and spin-polarizations whose fluctuations strongly increase as a system becomes less chaotic. The crucial features are illustrated with a model that depends on a parameter that tunes the dynamics from nearly integrable to mostly chaotic.

Our interest in this letter lies in microstructures fabricated using electrostatic gates or etching that pattern a two dimensional electron gas in a semiconductor heterostructure, for example, GaAs/AlGaAs. Typically, the electronic transport mean free path is significantly larger than the dimensions of the device, and the electrons essentially travel ballistically across the microstructure. Their motion is governed by the shape of a smooth, self-consistent, steep-walled, confining potential which is often conceptualized as a quantum billiard.

For many physical properties, the simplifying assumption that the dots’ underlying classical dynamics are fully chaotic (hard chaos) has provided a good description of the experimental data [1, 2, 3, 4]. It has been used to justify various hypotheses from the applicability of random matrix theory (RMT) and random plane wave modeling (RPW) to statistical assumptions applied within semiclassical mechanics [5, 6, 7]. Indeed, chaotic systems manifest a large variety of *universal* behaviors. Furthermore, chaotic quantum dots are often qualitatively very similar to diffusive ones provided the Thouless energy E_{TH} is defined as $\hbar v_F/L$, where v_F is the Fermi velocity and L is a typical dimension of the dot (as opposed to $\hbar D/L^2$ with D the diffusion constant). Consequently, most techniques, developed much earlier to study disordered metals (diagrammatic approaches [8], nonlinear sigma model [9]) and applied to disordered quantum dots [10, 11, 12], are applicable to ballistic quantum dots.

Nevertheless, unlike billiards, there are no known smooth potentials which are truly, fully chaotic. Unless designed otherwise for a specific purpose (such as measuring the weak localization lineshape [13]) an odd-shaped, smooth potential generically exhibits *soft* chaos, i.e. significant contributions of *both* stable and unstable motion. The general assumption of hard chaos is unfounded.

As opposed to a genuine belief that the electrons’ dynamics are strongly chaotic, the implicit assumption is that for many properties the distinctions between soft and hard chaos are more subtle than spectacular. This has been shown explicitly, for instance, for the fluctuation properties of Coulomb blockade (CB) peak heights [14], or for their correlations [15]. In such circumstances, using a chaotic model allows for simpler analytic derivations without drastically altering the results.

Our purpose here is to demonstrate that even this weaker

assumption may, in some cases, be problematic; and that for some properties or measurements a strong sensitivity to the nature of the dynamics arises. Because the distinction between the chaotic and integrable limits becomes most apparent at long (infinite) times, confining the electrons as long as practical within the dot holds the promise of leading to signatures of the dynamics. We shall therefore consider [zero temperature] ground states properties of well isolated dots, and find that ground state energies (whose second differences are probed by CB peak spacing measurements), and spin polarizations are markedly affected by the dynamics.

We proceed as follows. First, we give a general discussion of why, in principle, chaotic dots should be rather “atypical”, at least as far as ground state properties are concerned. Secondly, we consider in more detail a particular Hamiltonian model, namely a time-reversal non-invariant coupled quartic oscillator system, and show more quantitatively the relevance of the underlying dynamics.

In the following, we assume a Fermi-Landau liquid description of the quantum dot [10, 11, 16], and therefore that the ground state energy $E_{gr}[N]$ is the sum of three terms

$$E_{gr}[N] = \mathcal{E}_{TF} + \mathcal{E}_{1p} + \mathcal{E}_{ri} . \quad (1)$$

$\mathcal{E}_{TF}[N] = (eN)^2/2C$ is an electrostatic energy, $\mathcal{E}_{1p}[N]$ is the sum of the single particle energies (SPE) of N *independent* particles, and \mathcal{E}_{ri} is a residual interaction term. Specifically

$$\mathcal{E}_{1p}[N] = \sum_{i,\sigma} f_i^\sigma \epsilon_i , \quad (2)$$

with ϵ_i the SPEs corresponding to an effective potential $V_{eff}(\mathbf{r})$ (that can be determined self-consistently within the electrostatic-like approximation) and $f_i^\sigma = 0$ or 1 is the occupation number of orbital i with spin $\sigma = \pm 1$, ($\sum_{i,\sigma} f_i^\sigma = N$). Furthermore, denoting ψ_i the eigenstate associated to ϵ_i ,

$$\begin{aligned} \mathcal{E}_{ri} = & \frac{1}{2} \sum_{i,j,\sigma,\sigma'} f_i^\sigma f_j^{\sigma'} \int d\mathbf{r} d\mathbf{r}' |\psi_i(\mathbf{r})|^2 V_{sc}(\mathbf{r} - \mathbf{r}') |\psi_j(\mathbf{r}')|^2 \\ & - \frac{1}{2} \sum_{i,j,\sigma} f_i^\sigma f_j^\sigma \int d\mathbf{r} d\mathbf{r}' \psi_i(\mathbf{r}) \psi_j^*(\mathbf{r}) V_{sc}(\mathbf{r} - \mathbf{r}') \psi_j(\mathbf{r}') \psi_i^*(\mathbf{r}') \end{aligned}$$

is the direct-plus-exchange, first order perturbation contribution in terms of the weak screened Coulomb interaction V_{sc} .

For the experimentally relevant electronic densities, V_{sc} is a short range function, and we shall model it as

$$V_{\text{sc}} = \frac{\zeta}{\nu} \delta(\mathbf{r} - \mathbf{r}') \quad (3)$$

with ν the total density of states (including the spin degeneracy factor $g_s = 2$) and $\zeta \in [0, 1]$ a parameter that can be related to the density of electrons (i.e. the parameter r_s of the electron gas) and is in the range $[0.5, 0.8]$ for many experiments. Within this zero range approximation, the residual interaction contributions read

$$\mathcal{E}_{\text{ri}} = \zeta \frac{\Delta}{g_s} \sum_{i,j} f_i^{(+)} f_j^{(-)} M_{ij} \quad (4)$$

with Δ the (local) mean SPE spacing and

$$M_{ij} = A \int d\mathbf{r} |\psi_i(\mathbf{r})|^2 |\psi_j(\mathbf{r})|^2. \quad (5)$$

A is the dot area. The M_{ij} are dimensionless and semiclassical reasoning implies that their mean (for $i \neq j$) is unity.

Note the crucial point that in Eq. (4), only electrons with opposite spins actually interact. Aligning two spins decreases the residual interaction by a quantity of $O(\Delta)$. There is thus a competition between the SPE term, which favors the occupation of the lowest orbitals, and the residual interaction term, which tends to align the electron spins. The relative strength of these two effects is governed by the dimensionless parameter ζ . If $\zeta > 2$, the ground state is completely polarized. This is the well known Stoner instability [17], which for instance is responsible for the ferromagnetic character of cobalt.

Here ζ is just less than one. Although full polarization is excluded, the proximity of the Stoner instability makes the ground state spin very sensitive to the fluctuations of the M_{ij} and ϵ_i , which affects the fluctuation properties of the ground state [7, 10, 11, 18]. This is sometimes referred to as the ‘‘mesoscopic Stoner fluctuation’’.

Now consider the diagonal term

$$M_{ii} = A \int d\mathbf{r} |\psi_i(\mathbf{r})|^4. \quad (6)$$

M_{ii} is the inverse participation ratio in position representation of the state ψ_i , which measures its extent of localization. Hard chaotic systems possess eigenfunctions that are the least localized in the sense that their Wigner transforms uniformly cover the energy surface [19]. However, mixed systems are known to display various forms of *phase space localization* [20]. This arises by various mechanisms. The most familiar one is associated with the quantization of invariant tori. It affects only a minority of states, but localizes them very strongly. Another mechanism discussed in [20] is associated with the presence of partial transport barriers in phase space, the presence of which should be quite typical in mixed dynamical systems. Such partial barriers, if they are effective, should affect almost all eigenstates, but produce a lesser degree of localization.

Similarly, it can be shown that the mean value of the off-diagonal terms $M_{i,j \neq i}$ should be independent of the dynamics, and their fluctuations are extremely small for chaotic systems (vanishing in the semiclassical limit [7]). However, they would be of $O(\Delta)$ if significant phase space localization is present. We therefore see that chaotic systems, rather than behaving *typically*, are rather the limiting class of systems for which the interaction is the *least* effective.

To explore the affect of soft chaos on the ground state properties, we introduce a specific model. Let the effective Hamiltonian \hat{H}_{eff} resulting from the lowest order, electrostatic-like, self-consistent calculation be ($\mathbf{r} = (x, y)$, $r = |\mathbf{r}|$)

$$\hat{H}_{\text{eff}} = \frac{(\mathbf{p} - \kappa \sqrt{a(\lambda)} x^2 \frac{\mathbf{r}}{r})^2}{2} + a(\lambda) \left(\frac{x^4}{b} + by^4 + 2\lambda x^2 y^2 \right). \quad (7)$$

Weyl operator ordering is assumed for the quantized version. The parameter $b = \pi/4$ is introduced so that the system has the symmetry of the rectangle instead of the square. $a(\lambda)$ is a convenient scaling factor chosen so that the mean number of states with energy smaller than E is given by $N(E) = E^{3/2}$, regardless of the choice of λ or κ . λ is the coupling between the oscillators. Finally, the parameter κ breaks time reversal invariance (TRI). Note that for TRI systems, higher order terms in the ground state energy expansion, in particular the Cooper series, should be taken into account. Therefore, κ is chosen such that TRI is completely broken. The specific form of the TRI breaking term has been chosen not to pertain to any particular physical realization, but to insure that the phase space portrait of the dynamics does not depend on the energy. By choosing λ and κ appropriately, various regimes of dynamics can be studied. In particular, we consider $(\lambda, \kappa) = (+0.20, 1.00)$ [nearly integrable], $(-0.20, 1.00)$ [mixed], and $(-0.80, 1.00)$ [mostly chaotic]. Due to the TRI breaking term somewhat stabilizing the dynamics, the motion in the chaotic case is still not quite fully chaotic.

The reflection symmetries lead to four irreducible representations, which can be thought of as independent quantum dots with the same dynamics. We consider the four systems as an ensemble, which allows us to decrease our statistical ‘error bars’ in the calculations. In fact, we increase the size of the ensemble even more by allowing λ to vary ± 0.02 , which is enough to get nearly independent quantum eigenproperties, but small enough that the structure of the dynamics is essentially unchanged. Each statistical measure calculated within a given dynamical regime is thus the result of averaging over an ensemble of 12 similar quantum dots.

For each parameter set, it is possible to compute for each symmetry class ($e_x = \pm 1, e_y = \pm 1$) the eigenvalues ϵ_i and eigenvectors ψ_i , from which the residual interaction terms Eq. (5) can be deduced (see [21] for the numerical details). We first consider a few interesting statistical properties of these quantities, and afterward see how the spin distribution and ground state energy fluctuations are affected.

In Fig. 1, values of sets of diagonal terms M_{ii} are represented for the symmetry class $(+, +)$ in the various dynamical

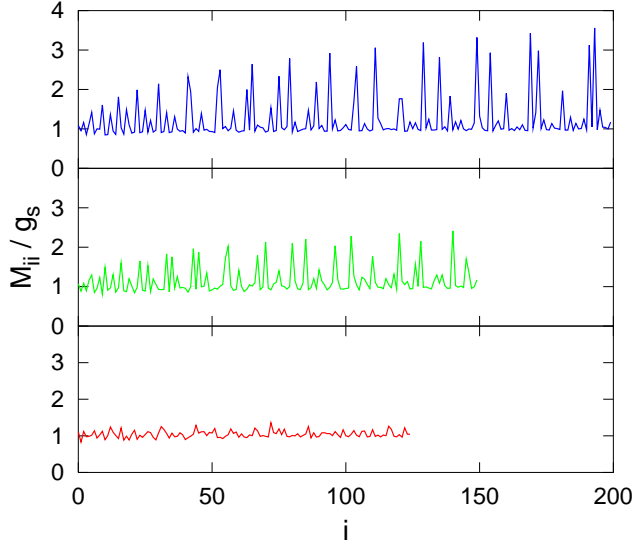


FIG. 1: Inverse participation ratio as a function of the orbital index for $(+, +)$. From top down: $(\lambda, \kappa) = (+0.20, 1.00)$ [nearly integrable], $(-0.20, 1.00)$ [mixed], and $(-0.80, 1.00)$ [mostly chaotic].

cal regimes. The presence of very localized states in the nearly integrable and mixed regimes is immediately apparent. Curiously enough, it turns out that for all dynamical regimes, the IPR M_{ii} is not very far from two for most states, but the distribution has a very long tail if the dynamics are not sufficiently chaotic. Consequently, it is reasonable to assume that the localization mechanism at work here is associated with stable periodic orbits or tori. A more detailed analysis of the classical dynamics reveals that partial barriers are actually present in $(\lambda, \kappa) = (-0.20, 1.00)$, but that their position with respect to the symmetry lines of the system make them ineffective in changing the statistics of the M_{ii} . Furthermore, and as can be seen in Table I, the off-diagonal terms M_{ij} ($i \neq j$) are also affected by eigenstate localization as their variance is significantly larger if the state i is localized.

The difference between the distribution of M_{ij} observed for the quartic oscillator system and that predicted for a chaotic system is essentially that a non-negligible number of very localized states ψ_i give much larger diagonal terms, and much larger variation of the corresponding off-diagonal terms. The

λ	+0.20	-0.20	-0.80
I^{sup}	2.0	1.8	1.2
I^{inf}	1.2	1.2	1.0
$M_{ii}/g_s > I^{\text{sup}}$	0.097	0.108	0.070
$M_{ii}/g_s < I^{\text{inf}}$	0.024	0.023	0.009

TABLE I: Conditional variance of the interaction terms M_{ij} with $0 < |i - j| \leq 10$, $i \geq 51$. Rows top down: i) dynamical case, ii) superior limit, iii) inferior limit, iv) conditional variance with localized orbitals, and v) conditional variance with delocalized orbitals.

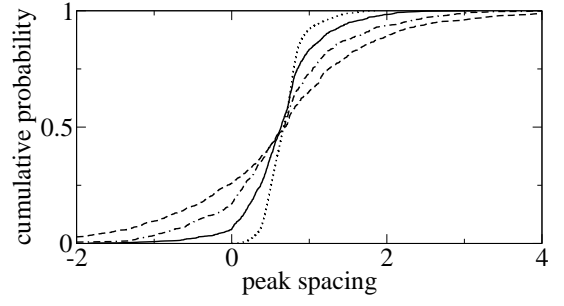


FIG. 2: Integrated peak spacing distribution with $\zeta = 0.8$ for RMT/RPW prediction [7] (dotted line), mostly chaotic (solid), mixed (dash-dot) and nearly integrable (dash) regimes.

question is how does this affect the ground state properties. The answer for given (λ, κ) and number of electrons in the dot N follows from the ϵ_i and M_{ij} . To compute the energy $E[\{f_i^\sigma\}]$, we use Eqs. (1,2,4) for the various occupations $\{f_i^\sigma\}$ such that $\sum_{i\sigma} f_i^\sigma = N$. The ground state follows by selecting the occupation sequence minimizing this energy. Varying N in the range $[100, 200]$ for each parameter set, one constructs a distribution of total spins, occupancies, and second differences in the ground state energy $\xi[N] = E_{\text{gr}}[N+1] + E_{\text{gr}}[N-1] - 2E_{\text{gr}}[N]$. $\xi[N]$ is experimentally accessible by measuring CB peak spacings, and we therefore refer to it as a “peak spacing”. The various dynamical regimes’ peak spacing distributions are shown in Fig. 2.

We see that the observed distributions are strikingly different from the RMT/RPW predictions (shown on the same plot) that should apply for fully chaotic systems. Even our most chaotic case shows significant deviations, and this increases considerably as the system moves away from hard chaos. The peak spacings fluctuate much more, and very large spacings appear for the mixed and nearly integrable regimes. Moreover, as shown in Table II, larger spins become significantly more probable.

We next ask how is such a drastic change made possible by the presence of a moderate number of very localized states. Let’s consider one specific example in detail. Fig. 3 shows the succession of orbital fillings for a range of N . Here, two of the single particle states ($i = 64, 66$), are highly localized. Since the system is not chaotic, there is also less level repulsion, which allows for the clustering of levels around ϵ_{64} or ϵ_{69} that

λ	+0.20	-0.20	-0.80	RMT/RPW
$P(s=2)$	0.13	0.16	0.07	0.01
$P(s=5/2)$	0.08	0.10	0.02	0.00
$\langle \delta s \rangle$	0.51	0.54	0.38	0.23

TABLE II: Probabilities $P(s=2)$, $P(s=5/2)$ to find a spin two (even N) or five halves (odd N) ground state, and average value $\langle \delta s \rangle$ of the ground state spin augmentation ($\delta s = s$ or $(s-1/2)$ for even or odd number of particles, respectively), for the various dynamical regimes (values of λ) with $\kappa = 1.0$ and $\zeta = 0.8$. The last column is the RMT/RPW prediction [7].

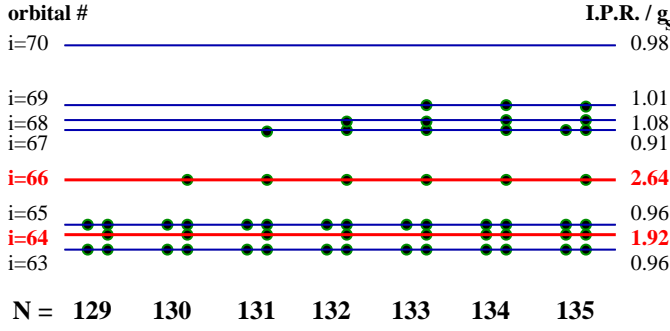


FIG. 3: Successive filling of the $(+, +)$ orbitals $i = 63$ to 69 as the number of particles in the dot goes from $N = 129$ to 135 for $(\lambda, \kappa) = (+0.20, 1.00)$ and $\zeta = 0.8$. The spacing between the horizontal lines are proportional to the actual level spacings. The numbers in the right column are the corresponding IPRs.

would otherwise be improbable. We see that none of the orbital occupations follow the simple “up/down” scenario characteristic of non-interacting systems. As would seem natural, the very localized orbitals $i = 64, 66$ remain singly occupied across many values of N . There is an additional non-intuitive feature, namely that the other orbitals also prefer single occupancy despite not being particularly localized.

This behavior derives from the following mechanism. Suppose for whatever reason, a given orbital i^* is singly occupied, say with spin $+$. The M_{ii^*} have to be included in the total energy for *all* orbitals i if $(i, -)$ is occupied, but not if only $(i, +)$ is. This can make the energy cost of occupying an orbital with spin down $(\zeta\Delta/g_s)$ higher than doing so with spin up. Assuming N_l such singly occupied orbitals already exist, and adding the term $(\zeta\Delta/g_s)M_{ii}$ associated with the interaction between the $(i, +)$ and the $(i, -)$ particles, on average it turns out that (even for a non-localized state) the residual interaction energy cost of doubly occupying some orbital i is $((N_l + 2)\zeta\Delta/g_s)$. For typical values of ζ , this is larger than a mean spacing as soon as $N_l \geq 1$. Consequently, as illustrated by Fig 3, the localized orbitals will not only remain singly occupied, but also have a tendency to polarize the electrons in the other nearby orbitals. Lack of level repulsion and larger fluctuations of the M_{ij} will further enhance such effects.

To conclude, we have shown that for the non-TRI quartic oscillators the eigenfunction statistics behave differently than those from a RMT/RPW approach. The significance is correlated with the degree of chaos (or lack thereof) in the underlying classical dynamics. Due to the proximity of the Stoner instability, strong effects arise in ground state spin polarizations, occupancies, and energies of the corresponding “model” quantum dot. The quartic oscillators more fairly represent a generic experimental dot than the hard chaos assumption. The hard chaos assumption leads to predictions that are qualitatively and quantitatively incorrect.

Finally, such considerations should affect the understanding of realized dots, which needs to be discussed on a case-by-case basis. For instance, the dots used in [22] are certainly far from chaotic. They should show a large degree of phase

space localization in their single particle properties, whereas this point is debatable with respect to the dots of [4]. However, it may be more interesting to address this question from the opposite point of view. Since creating dots away from the hard chaos limit leads to behaviors that are qualitatively different from those predicted using chaotic or diffusive modeling, if the interest is in devising a dot to perform some particular function, such as spin manipulation, for instance, it is in the soft chaos regime that richer behavior involving large fluctuations of ground state energies and spins will be found.

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- [1] R. A. Jalabert, A. D. Stone, and Y. Alhassid, Phys. Rev. Lett. **68**, 3468 (1992).
 - [2] A. M. Chang et al., Phys. Rev. Lett. **76**, 1695 (1996); J. A. Folk et al., Phys. Rev. Lett. **76**, 1699 (1996).
 - [3] G. Usaj and H. U. Baranger, Phys. Rev. **B 63**, 184418 (2001).
 - [4] S. R. Patel et al., Phys. Rev. Lett. **80**, 4522 (1998).
 - [5] O. Bohigas, M.-J. Giannoni, and C. Schmit, Phys. Rev. Lett. **52**, 1 (1984); M. V. Berry, J. Phys. A **10**, 2083 (1977).
 - [6] See e.g.: P. W. Brouwer, Y. Oreg, B. I. Halperin, Phys. Rev. **B 60**, 13977 (1999); P. W. Brouwer, J. N. H. J. Cremers, B. I. Halperin, Phys. Rev. **B 65**, 081302 (2002); Y. Alhassid, Rev. Mod. Phys. **72**, 89q5 (2000); K. Held, E. Eisenberg, B. L. Altshuler, cond-mat/0208177.
 - [7] D. Ullmo and H. U. Baranger, Phys. Rev. **B 64**, 245324 (2001).
 - [8] For a review see B. L. Altshuler and A. G. Aronov, in “Electron-Electron Interactions in Disordered Systems”, edited by A. L. Efros and M. Pollak, (North-Holland, Amsterdam, 1985).
 - [9] K. B. Efetov, “Supersymmetry in Disorder and Chaos”, (Cambridge University Press, 1996).
 - [10] Y. M. Blanter, A. D. Mirlin, and B. A. Muzykantskii, Phys. Rev. Lett. **78**, 2449 (1997).
 - [11] I. L. Aleiner, P. W. Brouwer, and L. I. Glazman, Phys. Rep. **358**, 309 (2002).
 - [12] P. N. Walker, G. Montambaux, and Y. Gefen, Phys. Rev. **B 60**, 2541 (1999); P. Jacquod and A. D. Stone, Phys. Rev. **B 64**, (2001) 214416.
 - [13] H. U. Baranger, R. A. Jalabert, and A. D. Stone, Phys. Rev. Lett. **70**, 3876 (1993); Chaos **3**, 665 (1993); A. M. Chang, et al., Phys. Rev. Lett. **73**, 2111 (1994).
 - [14] R. O. Vallejos, C. H. Lewenkopf, and E. R. Mucciolo, Phys. Rev. **B 60**, 13682 (1999).
 - [15] E. E. Narimanov, et al., Phys. Rev. Lett. **83**, 2640 (1999); Phys. Rev. **B 64**, 235329 (2001).
 - [16] D. Ullmo et al., Phys. Rev. **B 63**, 125339 (2001)
 - [17] E. C. Stoner, Rep. Prog. Phys. **11**, 43 (1947).
 - [18] I. L. Kurland, I. L. Aleiner, and B. L. Altshuler, Phys. Rev. **B 62**, 14886 (2000).
 - [19] N. L. Balazs and B. K. Jennings, Phys. Rep. **104**, 347 (1984).
 - [20] O. Bohigas, S. Tomsovic, and D. Ullmo, Phys. Rev. Lett. **65**, 5 (1990); Phys. Rep. **223**, 43 (1993).
 - [21] T. Nagano, D. Ullmo, and S. Tomsovic, to be published; T. Nagano, Ph. D. thesis, Washington State University, (2002).
 - [22] S. Lüscher et al., Phys. Rev. Lett. **86**, 2118 (2001).